

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SGGSB2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: SGGSB2

Bond precision: C-C = 0.0047 Å

Wavelength=0.71073

Cell: a=8.4186(11) b=8.9416(12) c=18.146(2)
 alpha=91.984(6) beta=97.826(6) gamma=117.594(5)

Temperature: 150 K

	Calculated	Reported
Volume	1191.9(3)	1191.8(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H39 B3 Ru2 S	C21 H39 B3 Ru2 S
Sum formula	C21 H39 B3 Ru2 S	C21 H39 B3 Ru2 S
Mr	558.15	558.15
D _x , g cm ⁻³	1.555	1.555
Z	2	2
Mu (mm ⁻¹)	1.359	1.359
F000	568.0	568.0
F000'	563.30	
h, k, l _{max}	10, 11, 23	10, 11, 23
N _{ref}	5483	5424
T _{min} , T _{max}	0.805, 0.885	0.732, 0.885
T _{min} '	0.805	

Correction method= # Reported T Limits: T_{min}=0.732 T_{max}=0.885
AbsCorr = MULTI-SCAN

Data completeness= 0.989

Theta (max)= 27.497

R(reflections)= 0.0268(4792)

wR₂(reflections)=
0.0638(5424)

S = 1.121

N_{par}= 273

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

● **Alert level C**

PLAT303_ALERT_2_C	Full Occupancy Atom H223	with # Connections	2.00	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	14	Report

● **Alert level G**

PLAT303_ALERT_2_G	Full Occupancy Atom H22A	with # Connections	2.00	Check
PLAT303_ALERT_2_G	Full Occupancy Atom H23A	with # Connections	2.00	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C6	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C20	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta (Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	45	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		4	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

